

# ADVANCED COMPUTATIONAL TECHNIQUES FOR MATERIALS-BY-DESIGN

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## Abstract

Modeling of uncertainty propagation in multi-scale models of deformation is extremely complex considering the nonlinear coupled phenomena that need to be accounted for. The ongoing work addresses key mathematical and computational issues related to robust control of deformation processes. Our research accomplishments for this year include development of new mathematical models based on spectral polynomial chaos, support space, and entropy maximization techniques for modeling sources of uncertainties in material deformation processes. These models, in conjunction with multi-scale models, allow simulations of the effect of microstructural variability on the reliability of macro-scale systems. We have developed the first stochastic variational multi-scale simulator with explicit sub-grid modeling, and a robust deformation process simulator for simulating uncertainties in metal forming processes. The non-intrusive stochastic Galerkin method developed as a part of the deformation simulator provides highly accurate estimates of the statistical quantities of interest within a fraction of time required using existing Monte-Carlo methods, and with minimal modification of existing deterministic software. The technique has also been applied to enable stochastic optimization of deformation processes. Finally, an information theoretic framework to capture microstructural uncertainties and its effect on macro-scale properties is summarized.

## 1 Status of effort

Substantial progress has been made in the achievement of this AFOSR-Comp Math project objectives in the 3<sup>rd</sup> year of this project. Key developments are listed below:

- Development of non-intrusive stochastic Galerkin method for robust modeling of deformation processes[1][2]
- Development of continuum stochastic sensitivity method (CSSM) for robust optimization of forming processes[2]
- Development of stochastic variational multi-scale model with explicit subgrid modeling for solving multi-scale partial differential equations (PDEs) in random heterogeneous microstructures [3][4]
- Development of maximum entropy techniques for modeling topological uncertainties in polycrystalline metallic microstructures and its influence of homogenized properties [5]

Particular contributions are briefly summarized below with more details given in the provided references.

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### 1.1 Development of a stochastic framework for analysis of metal forming processes

Two distinct approaches are being followed towards modeling uncertainties in deformation processes. In the first technique, Spectral Stochastic Finite Element Method (SSFEM), a spectral expansion of the current configuration of a deforming body is proposed using Legendre chaos expansions to compute the stochastic deformation gradient which is in turn used to compute statistics of several critical fields in large deformation analysis. A stochastic large deformation analysis following this approach is presented in our work in [6]. The second algorithm is based on a finite element representation of the support space of the random variables. This method is particularly useful for capturing instabilities and bifurcations in physical phenomena as demonstrated in [7]. The support space representation can lead to a non-intrusive decoupled as well as intrusive coupled formulation for evaluating the stochastic process. The highlight of the decoupled approach, called Non-Intrusive Stochastic Galerkin (NISG) method, is that it can be directly applied to presently available deterministic codes with minimal effort needed to compute the complete probability density function (PDF) of a stochastic process. In NISG method, the stochastic process is represented over the support space using piecewise continuous orthogonal polynomials in multi-dimensional random variables. The polynomials we choose are locally supported element shape functions used for representing functions in the finite element method. The  $h$  and  $p$  convergence characteristics of the discretized stochastic domain are identical to spatial finite elements.

In Fig. 1, we show a simulation of an isothermal, extrusion operation with a die of average diameter reduction of 14% [1]. The objective of the problem is to ascertain the effect of uncertain die geometry on the steady state distribution of the state variable at the exit. A 9x9 grid is used to discretize the support space. The mean and standard deviations of the state variable distribution at the die exit are plotted in Fig. 1(b&c) respectively. For this problem, NISG method provides highly accurate estimates of the statistical quantities of interest within a fraction of the time required using existing Monte Carlo methods. Our current effort focuses on adaptive methods based on sparse grid interpolants (variants of Smolyak algorithm) to efficiently represent stochastic quantities in large dimensional spaces. This development will allow inclusion of microstructural uncertainties during design of processes and allow reliability assessment in multi-scale models.

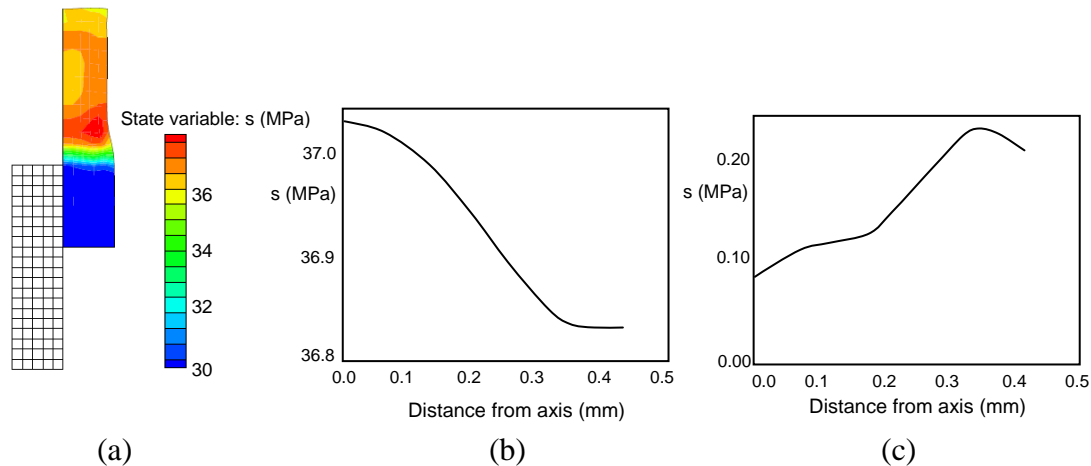


Fig. 1 (a) Initial and final mean configurations for the isothermal extrusion problem (b) Mean and (c) standard deviation of the state variable at die exit [1]

## 1.2 Stochastic optimization of metal forming processes

We have developed formulations for stochastic optimization of metal forming processes based on the continuum stochastic sensitivity method (CSSM)[2]. In deterministic design problems [8], the sensitivities of the various fields are computed in a mathematically rigorous approach by computing the derivatives of the governing equations with respect to the design variables using a predefined perturbation. An example of a deterministic forging design (with remeshing) for a 3D steering link is shown in Fig. 2 [2].

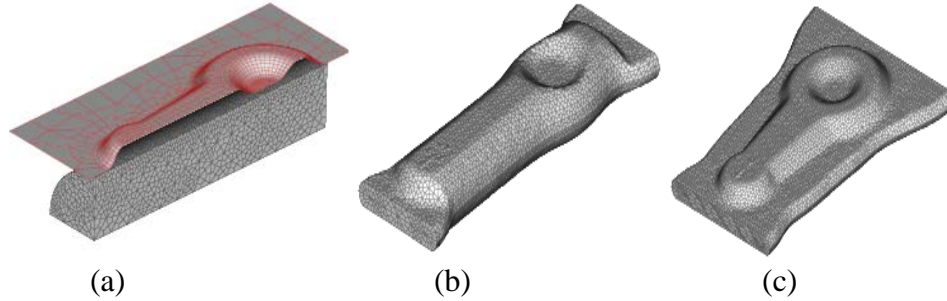


Fig. 2 (a) Die-workpiece setup for the steering link forging deterministic optimization problem (b) the final (under-filled) forged product of the initial design (c) Final forged product with optimized perform that minimizes flash and fully fills die cavity [2].

On the other hand, the objective of the *stochastic* optimization scheme is to undertake process design in the presence of uncertainty, i.e. in the optimization process, desired values of the properties in the objective function are also assumed to be random. Here, the aim is to compute the predefined random process design parameters which lead to desired objectives with given robustness limits in the final product. In the preform design problem that we consider (Fig. 3(a)), the preform shape is optimized to minimize barreling in the axisymmetric open die forging. We consider randomness being introduced as a result of uncertainty in the die-workpiece friction coefficient. We also assume that there is some uncertainty in the desired optimal shape. i.e. the design criteria is stochastic. The preform shapes for the stochastic solution (Fig. 3(b)) differs considerably from the deterministic optimal solution which emphasizes the need for robust design methods.

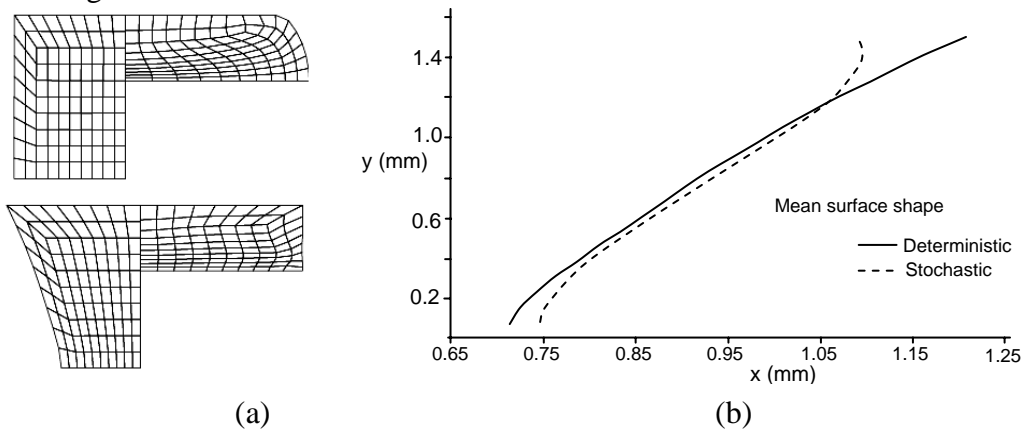


Fig. 3 (a) Initial (top) and final (bottom) configurations of the stochastic open die forging problem (b) Mean optimal preform shape in the deterministic and stochastic optimization problems [2]

### 1.3 Development of a stochastic variational multi-scale model with explicit sub-grid modeling

The focus of this work is to model uncertainty induced by micro-scale variability on the macro-scale outcomes. We have developed mathematical models for direct incorporation of the inherent randomness and the effect of modeling assumptions in the design of upscaling methods. The potential applications for the problem include solving PDEs in random heterogeneous microstructures, which is our key problem of interest. Using deterministic upscaling techniques for statistical analysis of the solution typically involves the use of computationally expensive Monte Carlo methods. In our work, we combine the variational multi-scale (VMS) method, the multi-scale finite element method and the GPCE approach to derive a variationally consistent upscaling technique [3][4]. Since randomness is effectively seen as an additional dimension in the problem, our method essentially performs upscaling for a class of problems corresponding to various realizations of the random material data.

As an example, a stochastic variational multi-scale formulation was used for addressing transient diffusion problems in random heterogeneous microstructure (Fig. 4(a)) with the stochastic parameter being the diffusion coefficient having multiple length scales. The main idea here was to calculate the diffusion dynamics on a highly coarse-mesh by including localized solutions to sub-grid problems. The method captures the mean field (Fig. 4(b)) as well as statistical quantities such as the first order fluctuations (Fig. 4(c)) in the temperature field in a single simulation.

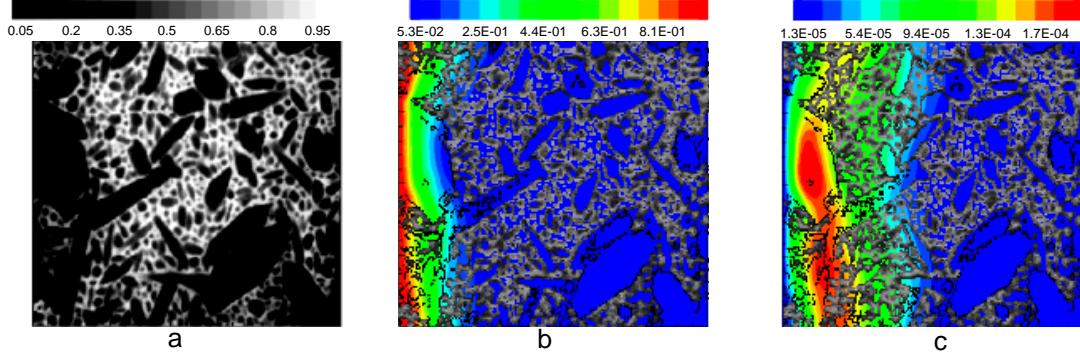


Fig 4. Modeling diffusion in heterogeneous random microstructures using a variational multi-scale algorithm: (a) Microstructure image realization, (b) Mean temperature field (coefficients  $u_0$  of GPCE), (c) First-order statistics (coefficient  $u_1$  in the GPCE) [3]

### 1.4 Information-theoretic microstructure reconstruction from available statistical information

This work allows us to mathematically represent statistics of micro-scale properties for use in multi-scale models. We utilize an information theoretic approach for computing bounds in plastic properties of metallic polycrystals [5]. Microstructures are treated as realizations of a PDF (probability density function). A particular problem of interest addressed here is the determination of effective behavior of polycrystalline materials based on uncertainties induced due to randomness in geometrical size and texture of microstructures. In obtaining the distribution from which microstructures are sampled, we

use the principle of maximum entropy (MaxEnt). Based on lower moments of grain sizes, we generate a distribution of grain sizes and this is compared with the grain size distribution of a representative microstructure as shown in Fig. 5(b). An example of randomness in properties induced by variability in grain sizes captured by MaxEnt algorithm is shown in Fig. 5(c). Key steps involved in this approach are:

- Downscaling of coarse-scale quantities: Statistics at the fine scale are constructed from averaged quantities (lower order moments such as mean grain size) at the macro-scale.
- Evaluating statistics of non-linear properties at the macro-scale using homogenization schemes developed recently [9]. Microstructure samples obtained from the PDF are represented using Voronoi tessellations (Fig. 5(a)).

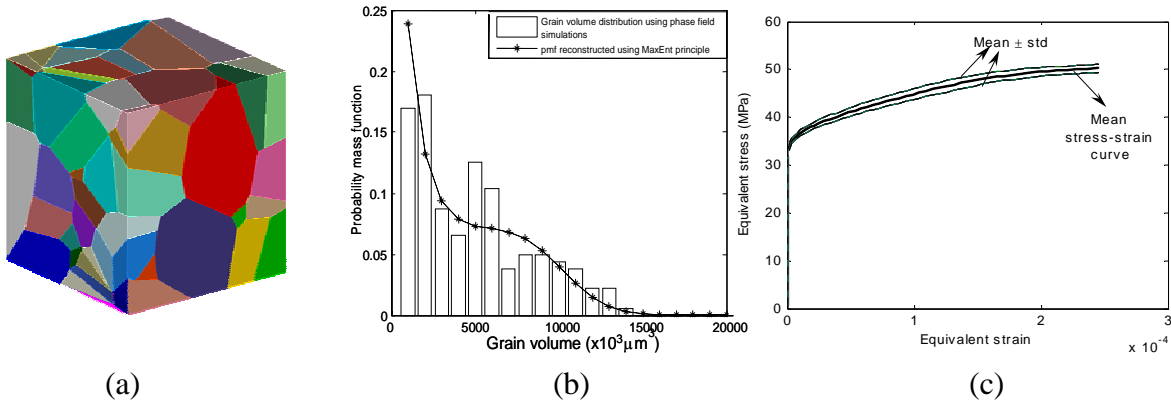


Figure 5 (a) A microstructure which is reconstructed based on the grain size distribution computed using MaxEnt (b) Comparison of grain size distribution obtained using MaxEnt and that of simulated microstructure (c) Mean and standard deviation of stress-strain curves obtained using homogenization techniques [5]

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### **Publications**

All archival publications are listed in the references above. Conference presentations and proceedings publications for 2005-06 are available for download at <http://mpdc.mae.cornell.edu/Publications/unrefereedConferences.htm>

### **Honors & Awards Received**

ASME Fellow—awarded April 2006

### **AFRL Point of Contact**

This work is being communicated with the AFRL group of Dr. R. Dutton AFRL/MLLM.

### **Transitions**

While no immediate commercialization plans are in place for the developed computational mathematics technologies, we strongly believe that their transition to immediate needs of DoD and industrial partners is forthcoming. As an indication, 2006 Army's Small Business Technology Transfer ([STTR](#)) Program solicitation # [A06-T009 Performance Map for Low-Cost Titanium Armor](#) has listed our work on statistical exploration of process/property/structure relations as one of the two key references.

### **New Discoveries**

(a) The first stochastic variational multi-scale algorithm with explicit subgrid modeling reported; (b) The first techniques reported for full-probabilistic modeling and design of deformation processes (c) New techniques for reconstruction of 3D microstructures from limited statistical information (d) Techniques for computing property variabilities due to topological uncertainties in the microstructure.